

Appendix A

```

    <?xml version="1.0" encoding="UTF-8" ?>
- <model name="FieldKorosNoyesModel">
- <notes>
5 <h1>Field-Koros-Noyes Model of BZ Reaction</h1>
- <table border="0" cellspacing="0" cellpadding="2">
- <thead>
- <tr>
    <th align="left" valign="middle" bgcolor="#eeeeee">Citation</th>
10 </tr>
    </thead>
- <tbody>
- <tr>
- <td>
15 <b>R.J.Field and R.M.Noyes,J.Chem.Phys.60,1877 (1974) ;
    R.J.Field,E.Koros,R.M.Noyes,JACS 94,8649 (1972);R.J.Field, R.M.Noyes,Nature
    237,390 (1972) This implementation is taken manufactured by J.D. Murray,
    "Mathematical Biology" (1989) page 181.
    <a href="" />
20 </td>
    </tr>
    </tbody>
    </table>
- <table border="0" cellspacing="0" cellpadding="2">
25 <thead>
- <tr>
    <th align="left" valign="middle" bgcolor="#eeeeee">Description</th>
    </tr>
    </thead>
30 <tbody>
- <tr>
    <td>Field Noyes Version of Belousov- Zhabotinsky Reaction. BrO3 is held
    constant; HOBr is typically ignored, and can be replaced by an empty- set. The
    stoichiometry f is typically taken as 1/ 2 or 1 (denominator 1 or 2 in SBML)
35 .</td>
    </tr>
    </tbody>
    </table>
- <table border="0" cellspacing="0" cellpadding="2">
40 <thead>
- <tr>
    <th align="left" valign="middle" bgcolor="#eeeeee">Rate constant    </th>
    <th align="left" valign="middle" bgcolor="#eeeeee">Reaction</th>
    </tr>
45 </thead>
- <tbody>
- <tr>
    <td>k1 = 1.3</td>
    <td>Br + BrO3 -> HBrO2 + HOBr</td>
50 </tr>

```

```

- <tr>
  <td>k2 = 2000000</td>
  <td>Br + HBrO2 -> HOBr^2</td>
</tr>
5 <tr>
  <td>k3 = 34</td>
  <td>BrO3 + HBrO2 -> Ce^2 + HBrO2^2</td>
</tr>
- <tr>
10 <td>k4 = 3000</td>
  <td>HBrO2^2 -> BrO3 + HOBr</td>
</tr>
- <tr>
  <td>k5 = 0.02</td>
15 <td>Ce -> Br^f</td>
</tr>
</tbody>
</table>
- <table border="0" cellspacing="0" cellpadding="2">
20 <thead>
- <tr>
  <th align="left" valign="middle" bgcolor="#eeeeee">Variable</th>
  <th align="left" valign="middle" bgcolor="#eeeeee">IC </th>
  <th align="left" valign="middle" bgcolor="#eeeeee">ODE</th>
25 </tr>
</thead>
- <tbody>
- <tr>
  <td>Br</td>
30 <td>0.003</td>
  <td>Br'[t] == -(k1*Br[t]*BrO3[t]) + f*k5*Ce[t] - k2*Br[t]*HBrO2[t]</td>
</tr>
- <tr>
  <td>Ce</td>
35 <td>0.05</td>
  <td>Ce'[t] == -(k5*Ce[t]) + 2*k3*BrO3[t]*HBrO2[t]</td>
</tr>
- <tr>
  <td>HBrO2</td>
40 <td>0.001</td>
  <td>HBrO2'[t] == k1*Br[t]*BrO3[t] - k2*Br[t]*HBrO2[t] +
    k3*BrO3[t]*HBrO2[t] - k4*HBrO2[t]^2</td>
</tr>
- <tr>
  <td>HOBr</td>
45 <td>0</td>
  <td>HOBr'[t] == k1*Br[t]*BrO3[t] + 2*k2*Br[t]*HBrO2[t]
    + k4*HBrO2[t]^2</td>
</tr>
50 </tbody>
</table>
</body>

```

```

    </notes>
- <listOfCompartments>
  <compartment name="BZ" />
</listOfCompartments>
5 <listOfSpecies>
  <specie name="Br" initialAmount="0.003" compartment="BZ" boundaryCondition="false"
    />
  <specie name="BrO3" initialAmount="0.1" compartment="BZ" boundaryCondition="true"
    />
10 <specie name="Ce" initialAmount="0.05" compartment="BZ" boundaryCondition="false"
    />
  <specie name="HBrO2" initialAmount="0.001" compartment="BZ"
    boundaryCondition="false" />
  <specie name="HOBr" initialAmount="0" compartment="BZ" boundaryCondition="false"
15 />
</listOfSpecies>
- <listOfReactions>
- <reaction name="Reaction1" reversible="false">
- <listOfReactants>
20 <specieReference specie="Br" />
  <specieReference specie="BrO3" />
  </listOfReactants>
- <listOfProducts>
  <specieReference specie="HBrO2" />
25 <specieReference specie="HOBr" />
  </listOfProducts>
- <kineticLaw formula="Br*BrO3*k1">
- <listOfParameters>
  <parameter name="k1" value="1.3" />
30 </listOfParameters>
  </kineticLaw>
  </reaction>
- <reaction name="Reaction2" reversible="false">
- <listOfReactants>
35 <specieReference specie="Br" />
  <specieReference specie="HBrO2" />
  </listOfReactants>
- <listOfProducts>
  <specieReference specie="HOBr" stoichiometry="2" />
40 </listOfProducts>
- <kineticLaw formula="Br*HBrO2*k2">
- <listOfParameters>
  <parameter name="k2" value="2000000" />
  </listOfParameters>
45 </kineticLaw>
  </reaction>
- <reaction name="Reaction3" reversible="false">
- <listOfReactants>
  <specieReference specie="BrO3" />
50 <specieReference specie="HBrO2" />
  </listOfReactants>
- <listOfProducts>

```

```

    <specieReference specie="Ce" stoichiometry="2" />
    <specieReference specie="HBrO2" stoichiometry="2" />
    </listOfProducts>
  - <kineticLaw formula="BrO3*HBrO2*k3">
5 <listOfParameters>
    <parameter name="k3" value="34" />
    </listOfParameters>
  </kineticLaw>
</reaction>
10 <reaction name="Reaction4" reversible="false">
  - <listOfReactants>
    <specieReference specie="HBrO2" />
    </listOfReactants>
  - <listOfProducts>
15 <specieReference specie="BrO3" />
    <specieReference specie="HBr" />
    </listOfProducts>
  - <kineticLaw formula="HBrO2^2*k4">
  - <listOfParameters>
20 <parameter name="k4" value="3000" />
    </listOfParameters>
  </kineticLaw>
</reaction>
  - <reaction name="Reaction5" reversible="false">
25 <listOfReactants>
    <specieReference specie="Ce" />
    </listOfReactants>
  - <listOfProducts>
    <specieReference specie="Br" stoichiometry="1" denominator="2" />
30 </listOfProducts>
  - <kineticLaw formula="Ce*k5">
  - <listOfParameters>
    <parameter name="k5" value="0.02" />
    <parameter name="f" value="0.5" />
35 </listOfParameters>
  </kineticLaw>
</reaction>
</listOfReactions>
</model>
40 </sbml>

```